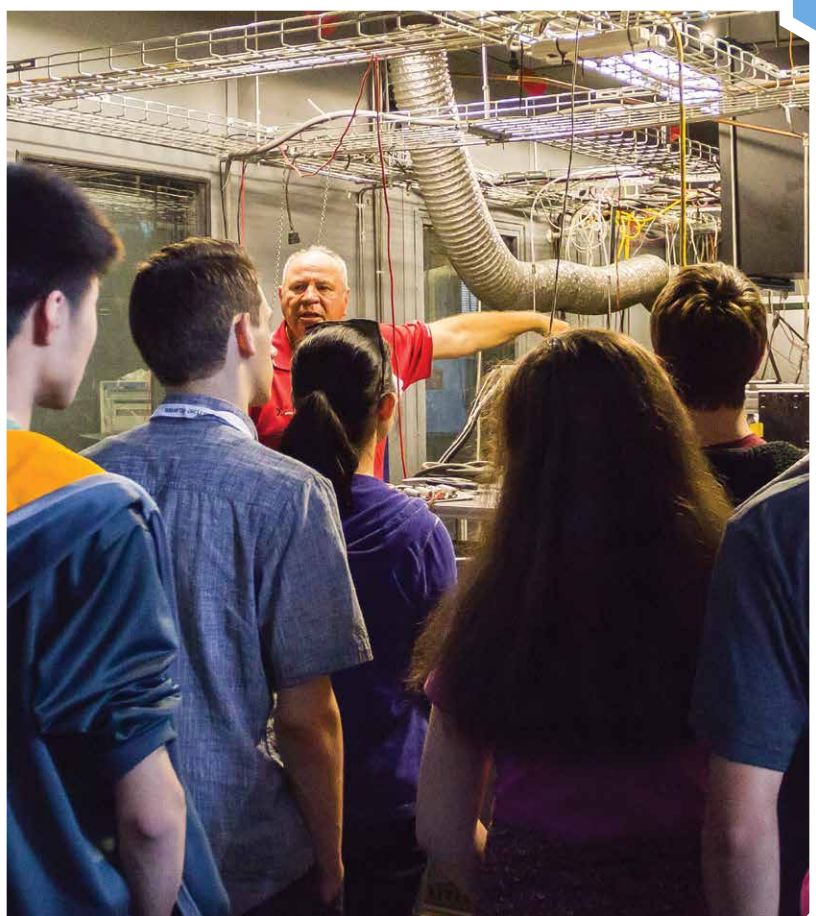
Ohio Supercomputer Center

An OH·TECH Consortium Member

Annual Report 2015–16



OSC Leadership:

David Hudak, Ph.D.
Interim Executive Director &
Director, Supercomputer Services
(614) 247-8670
dhudak@osc.edu

Alan Chalker, Ph.D.
Director, Technology Solutions &
Director, AweSim
(614) 247-8672
alanc@osc.edu

Basil Gohar
Manager, Web &
Interface Applications
(614) 688-0979
bgohar@osc.edu

Steven Gordon, Ph.D.
Senior Education Specialist
(614) 292-4132
sgordon@osc.edu

Brian Guilfoos
Manager, HPC Client Services
(614) 292-2846
guilfoos@osc.edu

Doug Johnson
Chief Systems Architect &
Manager, HPC Systems
(614) 292-6286
djohnson@osc.edu

Karen Tomko, Ph.D.
Interim Director of Research &
Manager, Scientific Applications
(614) 292-1091
ktomko@osc.edu

osc.edu

Chancellor John Carey directs the Ohio Department of Higher Education and oversees the strategic initiatives of the Ohio Technology Consortium and its member organizations in support of the state's technology infrastructure needs.

"The breadth and depth of OSC supercomputing services empower scientists to boost scientific discovery and engineers to foster industrial innovation across Ohio."

— *John Carey, Chancellor, Ohio Department of Higher Education*

OH·TECH | Ohio Technology Consortium
A Division of the **Ohio Department of Higher Education**

The Ohio Technology Consortium (OH-TECH) serves as the technology division of the Ohio Department of Higher Education and comprises a suite of technology and information member organizations unsurpassed in any other state: OSC, OARnet, OhioLINK and eStudent Services. Their consolidation under the OH-TECH banner allows each organization to pursue assorted synergies and efficiencies.

Ohio Supercomputer Center

The Ohio Supercomputer Center (OSC) addresses the rising computational demands of academic and industrial research communities by providing a robust shared infrastructure and proven expertise in advanced modeling, simulation and analysis. OSC empowers scientists with the services essential to making extraordinary discoveries and innovations, partners with businesses and industry to leverage computational science as a competitive force in the global knowledge economy and leads efforts to equip the workforce with the key technology skills required for 21st century jobs.

From the director

The Ohio Supercomputer Center is more than just large cabinets full of expensive hardware. We are a service organization that provides Ohio's university faculty, students, scientists and industry engineers with a wide range of services designed to deepen the impact of supercomputing on education and research across the state.

For example, many people find supercomputers too difficult to learn and too difficult to use. Our engineers have been working hard to provide new services and innovative tools, such as AweSim and OSC OnDemand, to make access to supercomputing simpler and more intuitive.

Also, OSC clients often lack the time or the skills to scale up their work and really use a supercomputer to its full capabilities. As a result, our hardware is too frequently "driven like a Ferrari in first gear." To address this, our staff members are increasingly focusing on client engagement, training, facilitation and software development.

Finally, to address the constantly rising demand for computing capacity, we installed a powerful new system in our data center. However, the Dell/Intel-Xeon Owens Cluster was just the beginning. We literally rebuilt our entire computing infrastructure, producing dramatic increases in all aspects of storage and interconnecting network speeds.

The point of all our improvements? To help keep Ohio among the leading states in scientific discovery and industrial innovation.

David Hudak, Ph.D.
Interim Executive Director

2015–16 highlights

Owens/infrastructure upgrades

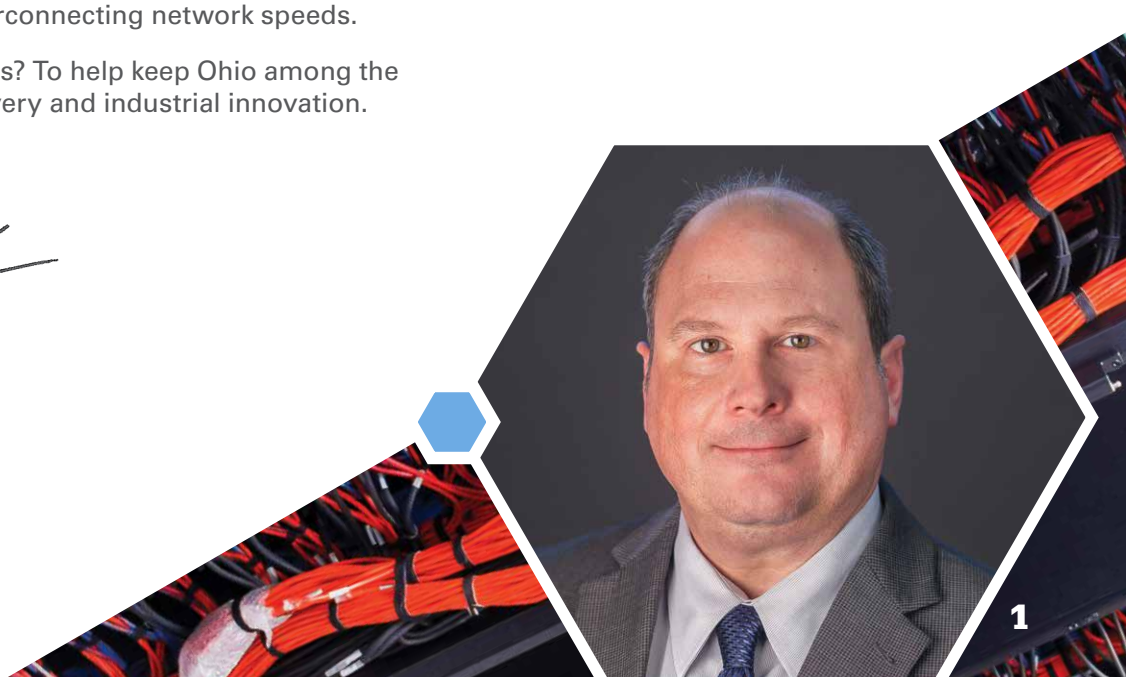
In 2015–16, OSC staff researched, purchased, received and installed the largest supercomputer system in the center's history. The Dell/Intel-Xeon Owens Cluster and related storage components increased total performance by a factor of four, while nearly tripling disk storage.

Supercomputer condo program

Efficiency is the keyword behind ongoing efforts to centralize supercomputing activity at OSC. Case in point, our engineers migrated researchers at the Ohio State Biomedical Informatics Department from a departmental-level computing system to a "condo" arrangement on our newest supercomputer systems, improving service while lowering costs.

Handling sensitive patient data

OSC engineers also deployed servers and software to support the Ohio State Division of Human Genetics in a pilot project to support sensitive patient data that can be analyzed with large-scale supercomputing resources.



Active Projects

New Project Investigators

Client Services

25 Ohio-based universities

33 companies

1,267 clients

124 trainees

10 training opportunities

451 awards made

459 projects served

19 academic courses used OSC's supercomputers

Production Capacity

161M+ core hours consumed

4M+ computational jobs

842 TB data stored

99.7% up-time (target: 96%)

Clients

While today's academic, health care and industrial researchers have many options for accessing HPC resources, each year more users turn to OSC as their partner in scientific discovery. With highly reliable educational computing services achieving 99.7 percent up-time this year, OSC continues to empower its clients as they break new ground in biosciences, advanced materials, manufacturing, energy and the environment along with a multitude of emerging disciplines.

Academic

This year, OSC served students, faculty and staff researchers across 25 universities. For 11 of these universities, 114 doctoral and 121 master's-level graduates used OSC in receiving their degrees. As a whole, OSC clients accomplished:

- 4 million computational jobs
- 161 million computing hours
- 451 projects launched by Ohio faculty
- 19 classroom projects

"Over the next five years, we're going to be using OSC computers to help us develop the tools that we're going to use to analyze WFIRST data when it arrives, and to define how the telescope needs to work in order to produce the science that we want."

— *David Weinberg, Ph.D., chair of the Department of Astronomy at The Ohio State University and researcher, NASA Wide Field Infrared Survey Telescope*

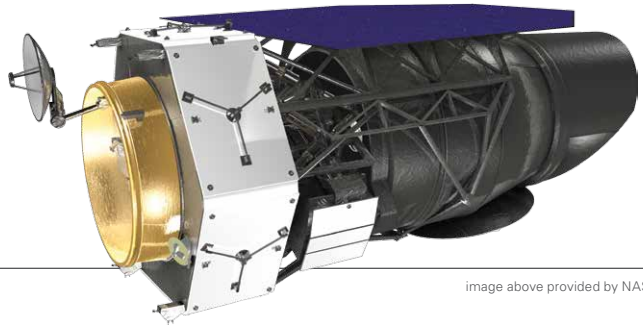


image above provided by NASA

Commercial

Under the AweSim program, OSC engineers, simulation and engineering experts and industry partners collaborate to provide small- to mid-sized manufacturers with simulation-driven design that enhances innovation and strengthens economic competitiveness. AweSim provides affordable, accessible and scalable modeling and simulation on high performance computers via:

- online modeling and simulation apps
- educational resources
- industry-specific expertise and consultants

From research involving auto racing to food processing, AweSim has continued to grow since its inception, with over 30 projects and 150 AweSim developers/clients, helping each to reduce prototyping time and costs. In fact, an industrial partner reported that for every $1 invested, modeling and simulation returned at least $7 on the investment.

"Without access to (OSC), what we do would be impossible. The money spent for us on CFD saves us money in the long run because when we go to the track and we go to the wind tunnel, we're already 90 percent sure that we're going down the right path."

— *Eric Jacuzzi, Senior Aerodynamics/Vehicle Performance Engineer, NASCAR*

Services/Training

OSC staff is poised to provide subject-matter experts from around the center to assist with individual client requests. For any issues that arise, OSC's 24/7 support desk, which now includes daytime Level 2 engineering support, is available to provide clients with technical expertise and consulting services at any hour of any day.

Cluster computing

OSC's cluster computing services provide resources to support high performance computing, high throughput computing and data-intensive computing. The new Owens Cluster, with its 23,000-plus cores and single-core scheduling, allows clients to run large parallel jobs, or large numbers of small independent calculations, in the same environment. Additionally, OSC has invested in special nodes as a part of the Owens purchase to give clients access to large shared-memory nodes, with large amounts of high-speed local storage, ensuring clients have access to the services they need to complete their research.

Client facilitation

Through the integration of increased training and education leadership over the past year, OSC is working toward deeper engagement with clients. OSC training and education leaders visited campuses this year to facilitate classroom projects, train students on the basics of supercomputing and demonstrate the broad service offerings OSC can provide. This takes an instructional load off faculty members so their time is maximized to focus on content and solving problems.

OSC also held a statewide curriculum meeting for users to discuss ways to improve the OSC classroom experience. OSC provided participants, representing 12 universities, with direct support, shared materials and instruction on AweSim and OnDemand interfaces, as well as various software packages. OSC also offers training and consultation for individual users to build core competencies for effective HPC use.

Software development

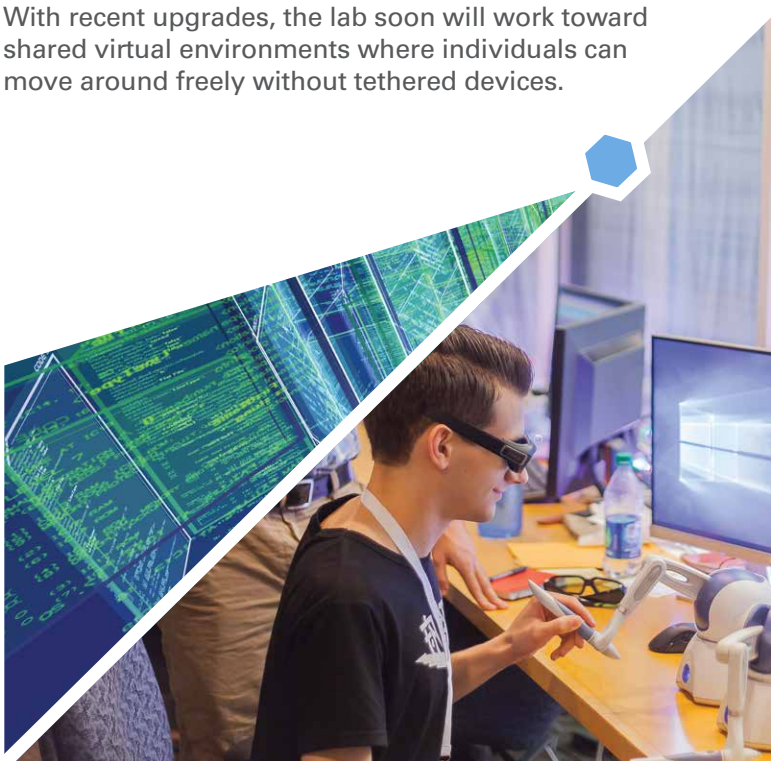
OSC provides ample access to software packages as well as the option for researchers to run software for which they provide the license, open source packages or in-house developed applications. OSC also offers a number of services related to scientific applications: optimization, parallelization, coding for GPU usage and more.

This summer, OSC debuted Open OnDemand, an open-source software based on the proven OSC OnDemand platform, to provide HPC centers around the U.S. and world the ability for their researchers and students to install and deploy advanced web and graphical interfaces.

For industrial clients, OSC's web and interface services team has allowed AweSim app developers to share apps through the AweSim dashboard, a mobile app store featuring client-developed resources. This makes modeling and simulation more affordable and accessible to even small businesses, as it requires little more than knowing how to use a website.

Visualization and virtual environments

OSC's award-winning Interface Lab translates technology into effective training and assessment tools for use by various sectors, such as the health care, automotive and manufacturing industries. With recent upgrades, the lab soon will work toward shared virtual environments where individuals can move around freely without tethered devices.



▶ OSC's Interface Lab uses advanced intuitive interfaces to integrate vast amounts of multisensory data into a single coherent simulation. Here, a student attending one of the Center's summer K–12 institutes (tour photo on front cover) works within a virtual environment, using haptic feedback technologies.

Systems/Owens

In 2016, OSC brought on board the most-powerful supercomputer in its history. Its name pays tribute to renowned Olympic sprinter, beacon for racial equality and youth advocate James C. "Jesse" Owens. Owens set or tied four collegiate world records in a single afternoon, sprinted to four gold medals and two Olympic records at the 1936 Berlin Games and dedicated much of his later life to helping youths overcome obstacles to their future success.

The Owens Cluster increases the center's total computing capacity by a factor of four. With $12 million in capital funds, the center not only brought in the new Dell/Intel Xeon cluster, but also upgraded and expanded disk storage by a factor of three with aggregate throughput performance of approximately 200 gigabits per second. Engineers also revamped infrastructure services to improve reliability and serviceability.

The new system is powered by Dell PowerEdge servers featuring the latest family of Intel® Xeon® processors, includes storage components manufactured by DDN and utilizes interconnects provided by Mellanox.

Additionally, the center provides more than 140 different software packages to researchers, with about 20 of them licensed packages. Researchers can bring their own licensed software, open-source packages or in-house developed applications, as well. Among the most-used software codes this past year were VASP for atomic scale materials modeling, OpenFOAM for computational fluid dynamics, LAMMPS for molecular dynamics simulation and MATLAB for numeric computation and visualization.

▶ The Owens Cluster, the most powerful computer OSC has ever run, arrived in June to the State of Ohio Computer Center.

High performance computing & storage

In 2015–16, approximately 1,300 researchers across Ohio depended on several key OSC systems:

Dell Intel Xeon Owens Cluster

23,392 cores provide a total peak performance of 750 teraflops

HP Intel Xeon Phi Ruby Cluster

4,800 cores provide a total peak performance of 144 teraflops

HP Intel Xeon Oakley Cluster

8,304 cores provide a total peak performance of 154 teraflops

DataDirect Storage System

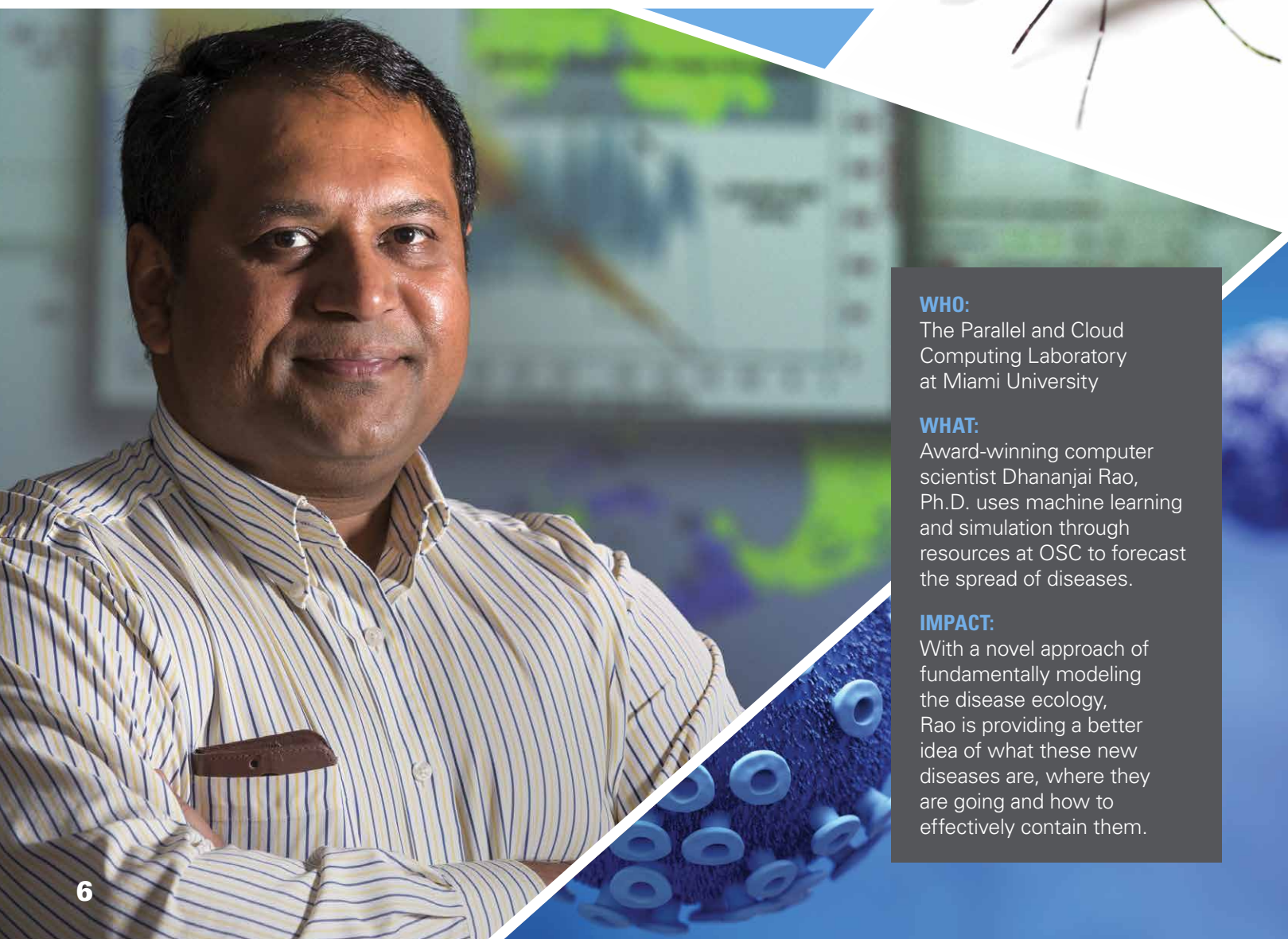
3.4 petabytes of high-performance spinning disk with 40–50 Gbps bandwidth

IBM Mass Storage System

5.5 petabytes of tape backup

Client Profile

Disease forecasting: New methodology will allow proactive approach to epidemic containment



WHO:
The Parallel and Cloud Computing Laboratory at Miami University

WHAT:
Award-winning computer scientist Dhananjai Rao, Ph.D. uses machine learning and simulation through resources at OSC to forecast the spread of diseases.

IMPACT:
With a novel approach of fundamentally modeling the disease ecology, Rao is providing a better idea of what these new diseases are, where they are going and how to effectively contain them.

When life-threatening weather events loom, forecasters warn citizens days, even weeks, beforehand so they can take action. It seems to work: We clear supermarket shelves, board up windows and even evacuate to higher ground ahead of the impending tempest to avoid danger.

Blind to bias in its threat to human life is another force of nature—epidemics.

Unfortunately, we often do not know they are imminent until the disease has already infiltrated an area. Dhananjai Rao, Ph.D., an assistant professor in the department of computer science and software engineering at Miami University, is using machine learning and simulation through resources at the Ohio Supercomputer Center (OSC) to apply the concepts of weather forecasting to epidemiology. He hopes this work will shift the paradigm for disease control from reactive to proactive.

"If we are able to forecast when, where and what an epidemic is going to be, then we can focus our energies and judiciously plan to mitigate the impact of those epidemics in those parts of the world so that the overall impact of the epidemic is significantly reduced," Rao said.

Rao has recently been studying mosquito-borne diseases, particularly chikungunya and the Zika virus. While there have been some efforts to forecast other known diseases, these existing methods rely on historical data trends to project the next stages of the disease. Unfortunately, for newly discovered diseases, such as the Zika virus, there is no historical data on which to base these statistical models.

"The gotcha with that is the statistical regression models will not be able to tell you what are the ecological processes that are happening. It can only tell you what is the final outcome of the system," Rao said. "Statistical (regression) models you can think of as a black box. You don't really understand what is going on inside."

Rao's approach of fundamentally modeling the disease ecology provides a better idea of what these new diseases are, where they are going and, from there, how to effectively contain them. To create a disease forecast, Rao layers data from multiple fields that collectively create the "perfect storm" of an epidemic. These include weather patterns, mosquito population and life cycle, human population density, air travel and socioeconomic data.

There are also critical parameters for which there are no known data, such as the probability that a mosquito will bite a human. To account for unknown parameters, Rao uses machine learning and parallel simulation to estimate these values. Rao leverages OSC's HP/Intel Xeon Oakley Cluster to study the overall ecology of a disease and how it propagates by looking at a combination of continuous and discrete event simulations.

This disease model analysis required 3.5 million simulations. This would take approximately 1,000 hours of CPU time, or about 90 days' work, on a single desktop computer.

"Three months. In three months, the epidemic would have long passed through the Americas, or the region that we're looking at," Rao said. "On Oakley, we were able to pull it off in about 12 hours, even at peak load."

Rao was one of 11 teams or individuals recognized recently in a competition organized by the U.S. Department of Defense's Defense Advanced Research Projects Agency (DARPA). The competition, known as the CHIKV Challenge, seeks to accelerate the development of new infectious disease forecasting methods. With help from Rao's groundbreaking model, DARPA as well as other government agencies can begin to look at how to mitigate the spread and effect of infectious diseases.

The next step of the process will involve advising health interventions and public policies to help contain epidemics. Rao said these policies will differ depending on the region and timing of the disease spread.

"There is not a day when we step out of the house without checking the weather, and that's where we want to go," Rao said. "For weather forecasting, it took about 100 years to come to where we are. With epidemic forecasting, we are hoping to be able to accelerate to where we want to be with supercomputing." •

"With epidemic forecasting, we are hoping to be able to accelerate to where we want to be with supercomputing."

— *Dhananjai Rao, Ph.D., Assistant Professor, Computer Science and Software Engineering, Miami University*

Client Profile

FSAE app helps student racing teams gain 'wind tunnel' access

During his 20-plus years in the high-stakes world of auto racing, Ray Leto rarely had time to offer much help to students interested in the engineering side of race teams.

When he became the president of TotalSim USA, Leto was able to make more time to mentor and advise students.

WHO:
TotalSim USA, an engineering services provider in Dublin, Ohio, and charter partner in the AweSim program at OSC.

WHAT:
TotalSim's FSAE app is a computational fluid dynamics (CFD) app for college students on Formula SAE (Society of Automotive Engineers) race teams.

IMPACT:
The app works as a virtual wind tunnel for the student-run team, giving them access to critical, previously unavailable, information to help in the development of their race cars.

One of the ways he's done that is by partnering with the Ohio Supercomputer Center (OSC) to help students help themselves with the FSAE app.

In late 2015, TotalSim USA—an engineering services provider in Dublin, Ohio, and charter partner in the AweSim program at OSC—developed a computational fluid dynamics (CFD) app for college students on Formula SAE (Society of Automotive Engineers) race teams. With the app, students can perform aerodynamics simulations on powerful OSC systems and get wind tunnel-like data for continued development of their racecars.

"The idea with this whole AweSim app ecosystem is to get modeling and simulation in the hands of people who normally couldn't afford it, or didn't have the time to become an expert," Leto said. "There's another avenue you can go down to get information, and this app is a great example of that."

AweSim is a public/private partnership, including OSC and modeling and simulation industry experts, working to provide manufacturers with competitive solutions for simulation-driven design.

Formula SAE is a competition amongst student-run teams in which a fictional manufacturing company has contracted a design team to develop a small Formula-style racecar. The teams design, build and test a prototype

"The idea with this whole AweSim app eco-structure is to get modeling and simulation in the hands of people who normally couldn't afford it, or didn't have the time to become an expert. There's another avenue you can go down to get information, and this app is a great example of that."

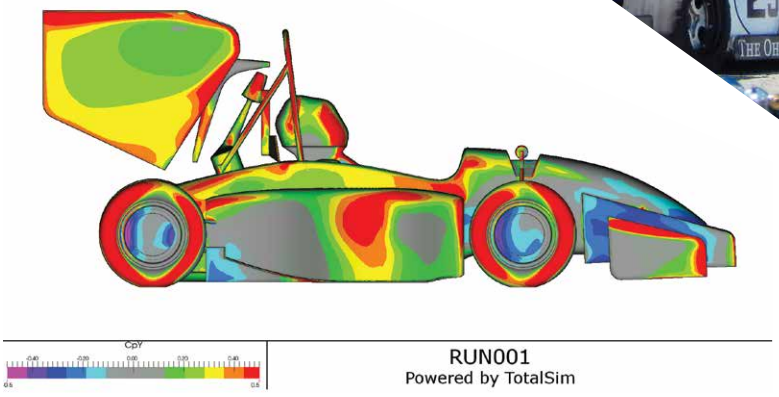
— *Ray Leto, president of TotalSim USA*

based on a series of rules aimed at promoting safety and testing problem solving skills.

The app itself renders geometric shapes into a mesh, configures solver settings, generates output visualizations and organizes results so students can focus on designing and improving their Formula SAE cars without first being forced to become CFD experts.

Three Formula SAE teams, including The Ohio State University, the University of Akron and Indiana University–Purdue University Indianapolis, have used the app, while UNC Charlotte and the University of Southern California teams have accounts.

"It's extremely easy to use," said Max Taylor, who recently graduated from Ohio State with a degree in aerospace engineering. "It's great for young engineers on an FSAE team because it allows them to experiment with designs and learn how to be an aerodynamicist without getting bogged down in code."



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Taylor was on OSU's Formula SAE team for three years, during which he was the aerodynamics team leader for two and was team captain his final year. Starting in the summer of 2015, Taylor became an intern at TotalSim and helped test and develop the FSAE app.

"The biggest benefit the app had for our team is it allowed us a solid foundation to begin the process each year," Taylor said. "When I joined the team, I had to more or less build our CFD capabilities from scratch. With me graduating this spring, our new aero team leader will have this app as a great starting point."

Andrew Borme, senior lecturer of motorsports engineering at IUPUI, said his students use the app for both the Formula SAE team and his aerodynamics class.

"It's invaluable because we don't have access to a wind tunnel or anything of that nature," Borme said. "With this system, each student got 10, 20, 30 runs per semester, and we were getting results, sometimes in a one-day turnaround. It was like Christmas every day."

Prior to the FSAE app, Borme said CFD testing was very limited or non-existent for student-run organizations. •

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1224 Kinnear Road | Columbus, OH 43212 | ph: (614) 292-9248